

Table S1. - Atomic coordinates for the non-hydrogen atoms of compound 6.

Atom ----	x --	y --	z --
PdA	-0.23163(2)	-0.34396(2)	-0.46158(1)
PdB	0.10096(2)	-0.08675(2)	0.24483(1)
PdC	0.20355(2)	0.63271(2)	0.04641(1)
ClA	-0.33832(7)	-0.25145(7)	-0.55618(3)
ClB	-0.00908(7)	-0.16757(6)	0.16155(3)
ClC	0.36630(8)	0.51841(8)	0.11073(4)
N1A	-0.0072(2)	-0.3377(2)	-0.4955(1)
N2A	-0.1406(2)	-0.4318(2)	-0.38445(9)
N1B	0.3234(2)	-0.1357(2)	0.2225(1)
N2B	0.1941(2)	-0.0217(2)	0.31742(9)
N1C	0.0081(2)	0.5537(2)	0.08557(9)
N2C	0.0616(3)	0.7224(2)	-0.0102(1)
C1A	0.0544(3)	-0.2828(2)	-0.5513(1)
C2A	0.2005(3)	-0.2844(2)	-0.5645(1)
C3A	0.2886(3)	-0.3444(3)	-0.5187(2)
C4A	0.2270(3)	-0.4058(2)	-0.4612(1)
C5A	0.0790(3)	-0.4011(2)	-0.4505(1)
C6A	0.0026(3)	-0.4592(2)	-0.3904(1)
C7A	0.0657(3)	-0.5382(2)	-0.3415(1)
C8A	-0.0199(3)	-0.5845(3)	-0.2876(1)
C9A	-0.1640(3)	-0.5539(3)	-0.2818(1)
C10A	-0.2262(3)	-0.4745(2)	-0.3314(1)
C11A	-0.3782(3)	-0.4240(3)	-0.3322(1)
C12A	-0.4135(3)	-0.3832(3)	-0.4065(1)
C13A	-0.4863(4)	-0.5140(4)	-0.3012(2)
C14A	-0.3838(4)	-0.3166(3)	-0.2910(2)
C1B	0.3817(3)	-0.1909(3)	0.1709(2)

C2B	0.5283 (4)	-0.2205 (3)	0.1658 (2)
C3B	0.6164 (3)	-0.1928 (3)	0.2141 (2)
C4B	0.5559 (3)	-0.1376 (3)	0.2677 (2)
C5B	0.4100 (3)	-0.1087 (2)	0.2705 (1)
C6B	0.3363 (3)	-0.0464 (2)	0.3246 (1)
C7B	0.3993 (3)	-0.0145 (3)	0.3806 (1)
C8B	0.3154 (4)	0.0421 (3)	0.4275 (1)
C9B	0.1702 (4)	0.0678 (2)	0.4181 (1)
C10B	0.1095 (3)	0.0358 (2)	0.3616 (1)
C11B	-0.0414 (3)	0.0627 (2)	0.3398 (1)
C12B	-0.0803 (3)	-0.0305 (2)	0.2941 (1)
C13B	-0.1537 (4)	0.0665 (3)	0.3995 (2)
C14B	-0.0408 (4)	0.1846 (3)	0.2991 (2)
C1C	-0.0121 (3)	0.4716 (2)	0.1385 (1)
C2C	-0.1466 (3)	0.4349 (3)	0.1606 (1)
C3C	-0.2657 (3)	0.4811 (3)	0.1274 (2)
C4C	-0.2463 (3)	0.5625 (3)	0.0717 (1)
C5C	-0.1085 (3)	0.5995 (2)	0.0526 (1)
C6C	-0.0763 (3)	0.6906 (2)	-0.0040 (1)
C7C	-0.1755 (4)	0.7413 (3)	-0.0479 (2)
C8C	-0.1283 (4)	0.8275 (3)	-0.0975 (2)
C9C	0.0102 (5)	0.8601 (3)	-0.1022 (2)
C10C	0.1095 (4)	0.8064 (3)	-0.0575 (1)
C11C	0.2627 (4)	0.8384 (3)	-0.0512 (2)
C12C	0.3451 (4)	0.7327 (3)	-0.0123 (2)
C13C	0.3401 (5)	0.8698 (4)	-0.1205 (2)
C14C	0.2555 (5)	0.9455 (3)	-0.0097 (2)

Table S2. - Atomic coordinates for the non-hydrogen atoms of compound 7.

Atom	x	y	z
----	-	-	-
Pd	-0.00078(2)	-0.14571(2)	-0.08408(1)
Cl	-0.19579(8)	-0.26481(7)	-0.05873(6)
N1	0.1768(2)	-0.2555(2)	-0.0104(1)
N2	0.1833(2)	-0.0554(2)	-0.1071(1)
C1	0.1636(4)	-0.3542(2)	0.0396(2)
C2	0.2869(4)	-0.4208(3)	0.0806(2)
C3	0.4258(4)	-0.3870(3)	0.0695(3)
C4	0.4415(3)	-0.2864(3)	0.0174(2)
C5	0.3135(3)	-0.2218(2)	-0.0214(2)
C6	0.3169(3)	-0.1130(2)	-0.0789(2)
C7	0.4468(3)	-0.0735(3)	-0.1023(2)
C8	0.4420(3)	0.0286(3)	-0.1550(2)
C9	0.3087(3)	0.0906(3)	-0.1799(2)
C10	0.1796(3)	0.0478(2)	-0.1542(2)
C11	0.0372(3)	0.1168(2)	-0.1777(2)
C12	-0.1041(3)	0.0484(2)	-0.2255(2)
C13	-0.1565(3)	-0.0346(2)	-0.1574(2)
C14	-0.2272(4)	0.1412(3)	-0.2589(2)
C15	-0.0726(4)	-0.0199(3)	-0.3096(2)

Table S3. - Positional and thermal parameters for the hydrogen atoms of compound 6.

Atom ----	x -	y -	z -	B (Å ²) -----
H1A	-0.0069	-0.2400	-0.5839	4.82
H2A	0.2414	-0.2435	-0.6056	5.62
H3A	0.3926	-0.3439	-0.5263	5.97
H4A	0.2873	-0.4512	-0.4290	5.15
H5A	0.1678	-0.5599	-0.3453	5.11
H6A	0.0225	-0.6397	-0.2532	5.71
H7A	-0.2230	-0.5868	-0.2434	5.74
H8A	-0.4593	-0.4460	-0.4249	5.39
H9A	-0.4783	-0.3137	-0.4076	5.39
H10A	-0.4820	-0.5809	-0.3273	8.10
H11A	-0.4625	-0.5405	-0.2554	8.10
H12A	-0.5829	-0.4775	-0.3011	8.10
H13A	-0.3149	-0.2600	-0.3109	7.30
H14A	-0.4802	-0.2797	-0.2908	7.30
H15A	-0.3598	-0.3427	-0.2451	7.30
H1B	0.3203	-0.2105	0.1366	5.86
H2B	0.5687	-0.2606	0.1282	7.21
H3B	0.7193	-0.2117	0.2105	7.08
H4B	0.6153	-0.1193	0.3030	6.21
H5B	0.5017	-0.0316	0.3866	5.54
H6B	0.3578	0.0638	0.4672	5.95
H7B	0.1111	0.1082	0.4508	5.58
H8B	-0.1233	-0.0966	0.3212	4.58
H9B	-0.1481	0.0045	0.2619	4.58
H10B	-0.1548	-0.0102	0.4255	6.96
H11B	-0.1285	0.1253	0.4277	6.96

H12B	-0.2485	0.0867	0.3827	6.96
H13B	0.0297	0.1829	0.2614	6.26
H14B	-0.1357	0.2046	0.2825	6.26
H15B	-0.0157	0.2431	0.3276	6.26
H1C	0.0712	0.4374	0.1616	4.74
H2C	-0.1578	0.3767	0.1994	5.74
H3C	-0.3617	0.4567	0.1429	5.85
H4C	-0.3279	0.5934	0.0463	5.23
H5C	-0.2747	0.7176	-0.0443	6.58
H6C	-0.1956	0.8649	-0.1291	7.69
H7C	0.0408	0.9211	-0.1369	7.64
H8C	0.3962	0.6849	-0.0440	6.64
H9C	0.4136	0.7625	0.0156	6.64
H10C	0.3437	0.8018	-0.1459	10.49
H11C	0.2876	0.9351	-0.1446	10.49
H12C	0.4374	0.8922	-0.1146	10.49
H13C	0.2065	0.9243	0.0337	9.46
H14C	0.3525	0.9682	-0.0033	9.46
H15C	0.2027	1.0111	-0.0333	9.46

Parameters without esd were not refined.

Table S4. - Positional and thermal parameters for the hydrogen atoms of compound 7.

Atom -----	x -	y -	z -	B(Å ²) -----
H1	0.0646	-0.3789	0.0469	5.12
H2	0.2749	-0.4909	0.1168	6.30
H3	0.5135	-0.4331	0.0978	6.68
H4	0.5395	-0.2617	0.0083	5.71
H7	0.5403	-0.1165	-0.0820	5.42
H8	0.5314	0.0566	-0.1744	6.13
H9	0.3049	0.1638	-0.2152	5.49
H111	0.0523	0.1812	-0.2187	4.67
H112	0.0180	0.1495	-0.1203	4.67
H131	-0.1950	0.0142	-0.1132	4.38
H132	-0.2369	-0.0832	-0.1923	4.38
H141	-0.2474	0.1846	-0.2058	5.80
H142	-0.1939	0.1963	-0.3012	5.80
H143	-0.3180	0.1013	-0.2906	5.80
H151	0.0052	-0.0787	-0.2887	5.59
H152	-0.1635	-0.0596	-0.3413	5.59
H153	-0.0394	0.0354	-0.3518	5.59

Parameter without esd were not refined.

Table S5. - Anisotropic thermal parameters (U's) for the non-hydrogen atoms of compound 6.

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
PdA	0.03980(8)	0.04604(9)	0.03780(8)	-0.00497(7)	-0.00673(7)	0.00346(7)
PdB	0.04352(8)	0.03872(8)	0.03608(8)	-0.00243(7)	-0.00636(7)	-0.00262(7)
PdC	0.0483(1)	0.04861(9)	0.03982(8)	-0.00461(8)	-0.00372(8)	-0.00561(8)
ClA	0.0551(3)	0.0706(4)	0.0495(3)	0.0000(3)	-0.0140(3)	0.0123(3)
ClB	0.0600(3)	0.0529(3)	0.0457(3)	-0.0055(3)	-0.0121(3)	-0.0091(3)
ClC	0.0468(3)	0.0898(5)	0.0697(4)	0.0041(4)	-0.0149(3)	-0.0007(4)
N1A	0.045(1)	0.0376(9)	0.0443(9)	-0.0057(8)	-0.0062(8)	0.0000(8)
N2A	0.046(1)	0.045(1)	0.0371(9)	-0.0084(8)	-0.0080(8)	0.0004(8)
N1B	0.048(1)	0.048(1)	0.051(1)	-0.0018(9)	-0.0031(9)	-0.0070(9)
N2B	0.052(1)	0.0398(9)	0.0383(9)	-0.0071(8)	-0.0059(8)	0.0002(8)
N1C	0.047(1)	0.045(1)	0.0387(9)	0.0035(9)	-0.0065(8)	-0.0067(8)
N2C	0.076(1)	0.039(1)	0.0374(9)	0.003(1)	-0.008(1)	-0.0032(8)
C1A	0.057(1)	0.043(1)	0.051(1)	-0.009(1)	-0.002(1)	0.003(1)
C2A	0.063(2)	0.052(1)	0.061(2)	-0.016(1)	0.007(1)	0.003(1)
C3A	0.048(1)	0.068(2)	0.073(2)	-0.011(1)	0.004(1)	-0.006(1)
C4A	0.044(1)	0.056(1)	0.064(1)	-0.004(1)	-0.007(1)	-0.005(1)
C5A	0.046(1)	0.037(1)	0.046(1)	-0.0062(9)	-0.008(1)	-0.0053(9)
C6A	0.045(1)	0.041(1)	0.043(1)	-0.006(1)	-0.0106(9)	-0.0044(9)
C7A	0.058(1)	0.049(1)	0.055(1)	-0.002(1)	-0.019(1)	0.000(1)
C8A	0.078(2)	0.053(1)	0.049(1)	-0.003(1)	-0.019(1)	0.009(1)
C9A	0.075(2)	0.063(2)	0.043(1)	-0.015(1)	-0.009(1)	0.006(1)
C10A	0.057(1)	0.056(1)	0.039(1)	-0.016(1)	-0.005(1)	0.001(1)
C11A	0.051(1)	0.072(2)	0.044(1)	-0.011(1)	0.001(1)	0.002(1)
C12A	0.044(1)	0.075(2)	0.050(1)	-0.006(1)	-0.003(1)	0.004(1)
C13A	0.068(2)	0.116(3)	0.068(2)	-0.032(2)	0.007(2)	0.016(2)
C14A	0.076(2)	0.095(2)	0.060(2)	0.008(2)	0.002(2)	-0.016(2)

C2B	0.070(2)	0.079(2)	0.077(2)	0.008(2)	0.015(2)	-0.012(2)
C3B	0.049(2)	0.082(2)	0.091(2)	0.002(2)	0.005(2)	-0.005(2)
C4B	0.049(1)	0.067(2)	0.080(2)	-0.007(1)	-0.005(1)	-0.003(2)
C5B	0.046(1)	0.046(1)	0.055(1)	-0.007(1)	-0.008(1)	0.002(1)
C6B	0.049(1)	0.043(1)	0.046(1)	-0.008(1)	-0.010(1)	0.003(1)
C7B	0.064(1)	0.053(1)	0.060(1)	-0.009(1)	-0.025(1)	0.003(1)
C8B	0.084(2)	0.059(1)	0.048(1)	-0.009(1)	-0.022(1)	-0.006(1)
C9B	0.085(2)	0.052(1)	0.042(1)	-0.005(1)	-0.010(1)	-0.009(1)
C10B	0.064(1)	0.037(1)	0.038(1)	-0.007(1)	-0.002(1)	-0.0023(9)
C11B	0.058(1)	0.045(1)	0.044(1)	0.001(1)	-0.001(1)	-0.005(1)
C12B	0.048(1)	0.049(1)	0.047(1)	-0.001(1)	-0.004(1)	-0.003(1)
C13B	0.075(2)	0.081(2)	0.064(2)	0.001(2)	0.012(2)	-0.021(1)
C14B	0.082(2)	0.046(1)	0.070(2)	0.004(1)	-0.016(2)	0.001(1)
C1C	0.053(1)	0.052(1)	0.044(1)	0.001(1)	-0.007(1)	-0.000(1)
C2C	0.063(2)	0.064(2)	0.052(1)	-0.005(1)	-0.002(1)	0.003(1)
C3C	0.048(1)	0.074(2)	0.064(2)	-0.004(1)	0.003(1)	-0.016(1)
C4C	0.046(1)	0.063(1)	0.059(1)	0.008(1)	-0.010(1)	-0.016(1)
C5C	0.053(1)	0.044(1)	0.043(1)	0.009(1)	-0.009(1)	-0.0138(9)
C6C	0.062(1)	0.044(1)	0.045(1)	0.010(1)	-0.009(1)	-0.010(1)
C7C	0.086(2)	0.062(2)	0.061(2)	0.020(2)	-0.022(1)	-0.008(1)
C8C	0.105(2)	0.070(2)	0.066(2)	0.021(2)	-0.024(2)	0.005(2)
C9C	0.134(3)	0.047(2)	0.057(2)	0.005(2)	-0.014(2)	0.011(1)
C10C	0.098(2)	0.046(1)	0.050(1)	-0.001(1)	-0.005(1)	-0.005(1)
C11C	0.103(2)	0.059(2)	0.062(2)	-0.021(2)	0.004(2)	-0.001(1)
C12C	0.075(2)	0.073(2)	0.064(2)	-0.020(2)	0.010(2)	-0.010(1)
C13C	0.136(3)	0.116(3)	0.077(2)	-0.043(3)	0.011(2)	0.016(2)
C14C	0.140(3)	0.062(2)	0.102(3)	-0.028(2)	-0.013(3)	-0.014(2)

The form of the anisotropic displacement parameter is:
 $\exp[-2\pi^2\{h^2a^2U(1,1) + k^2b^2U(2,2) + l^2c^2U(3,3) + 2hkabU(1,2) + 2hlacU(1,3) + 2klbcU(2,3)\}]$ where a, b, and c are reciprocal lattice constants.

Table S6. - Anisotropic thermal parameters (U's) for the non-hydrogen atoms of compound 7.

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Pd	0.03983(8)	0.03840(8)	0.03541(8)	-0.00157(8)	0.01229(6)	0.00316(8)
Cl	0.0503(3)	0.0572(4)	0.0832(4)	-0.0086(3)	0.0202(3)	0.0173(3)
N1	0.049(1)	0.045(1)	0.039(1)	0.0010(9)	0.0121(8)	0.0016(9)
N2	0.043(1)	0.0395(9)	0.0369(9)	-0.0031(9)	0.0113(8)	-0.0021(8)
C1	0.065(2)	0.049(1)	0.050(1)	0.001(1)	0.016(1)	0.008(1)
C2	0.081(2)	0.051(2)	0.064(2)	0.008(2)	0.008(2)	0.014(1)
C3	0.066(2)	0.065(2)	0.075(2)	0.017(2)	0.002(2)	0.011(2)
C4	0.052(2)	0.061(2)	0.067(2)	0.007(1)	0.009(1)	0.003(2)
C5	0.046(1)	0.044(1)	0.042(1)	-0.000(1)	0.009(1)	-0.002(1)
C6	0.043(1)	0.047(1)	0.042(1)	-0.005(1)	0.011(1)	-0.006(1)
C7	0.044(1)	0.066(2)	0.062(2)	-0.006(1)	0.012(1)	0.004(1)
C8	0.050(1)	0.075(2)	0.073(2)	-0.013(1)	0.020(1)	0.007(2)
C9	0.057(2)	0.057(2)	0.062(2)	-0.014(1)	0.018(1)	0.007(1)
C10	0.052(1)	0.041(1)	0.042(1)	-0.008(1)	0.013(1)	-0.002(1)
C11	0.058(1)	0.037(1)	0.055(1)	-0.001(1)	0.017(1)	0.003(1)
C12	0.052(1)	0.046(1)	0.037(1)	0.006(1)	0.013(1)	0.005(1)
C13	0.042(1)	0.050(1)	0.046(1)	0.005(1)	0.009(1)	0.009(1)
C14	0.067(2)	0.059(2)	0.059(2)	0.011(1)	0.015(1)	0.018(1)
C15	0.072(2)	0.066(2)	0.039(1)	0.006(2)	0.013(1)	-0.003(1)

The form of the anisotropic displacement parameter is:
 $\exp[-2\pi^2\{h^2a^2U(1,1) + k^2b^2U(2,2) + l^2c^2U(3,3) + 2hkabU(1,2) + 2hlacU(1,3) + 2klbcU(2,3)\}]$ where a, b, and c are reciprocal lattice constants.

Table S7. - Full list of bond distances and angles for compound 6.

Intramolecular Contacts

PDA	CLA	2.3207 ± 0.0010	(1 0 0 0)	
PDA	N1A	2.1548 ± 0.0019	(1 0 0 0)	
PDA	N2A	1.9623 ± 0.0019	(1 0 0 0)	
PDA	C12A	2.0033 ± 0.0026	(1 0 0 0)	
CLA	PDA	N1A	100.23 ± 0.10	(1 0 0 0) (1 0 0 0)
CLA	PDA	N2A	176.24 ± 0.10	(1 0 0 0) (1 0 0 0)
CLA	PDA	C12A	97.57 ± 0.10	(1 0 0 0) (1 0 0 0)
N1A	PDA	N2A	79.27 ± 0.10	(1 0 0 0) (1 0 0 0)
N1A	PDA	C12A	161.92 ± 0.10	(1 0 0 0) (1 0 0 0)
N2A	PDA	C12A	82.75 ± 0.10	(1 0 0 0) (1 0 0 0)
PDB	CLB	2.3056 ± 0.0010	(1 0 0 0)	
PDB	N1B	2.1465 ± 0.0021	(1 0 0 0)	
PDB	N2B	1.9668 ± 0.0021	(1 0 0 0)	
PDB	C12B	2.0116 ± 0.0025	(1 0 0 0)	
CLB	PDB	N1B	101.13 ± 0.10	(1 0 0 0) (1 0 0 0)
CLB	PDB	N2B	178.49 ± 0.10	(1 0 0 0) (1 0 0 0)
CLB	PDB	C12B	97.16 ± 0.10	(1 0 0 0) (1 0 0 0)
N1B	PDB	N2B	78.91 ± 0.10	(1 0 0 0) (1 0 0 0)
N1B	PDB	C12B	161.11 ± 0.10	(1 0 0 0) (1 0 0 0)
N2B	PDB	C12B	82.69 ± 0.10	(1 0 0 0) (1 0 0 0)
PDC	CLC	2.3079 ± 0.0010	(1 0 0 0)	
PDC	N1C	2.1354 ± 0.0020	(1 0 0 0)	
PDC	N2C	1.9676 ± 0.0022	(1 0 0 0)	
PDC	C12C	2.0206 ± 0.0032	(1 0 0 0)	
CLC	PDC	N1C	99.49 ± 0.10	(1 0 0 0) (1 0 0 0)
CLC	PDC	N2C	176.94 ± 0.10	(1 0 0 0) (1 0 0 0)
CLC	PDC	C12C	98.58 ± 0.10	(1 0 0 0) (1 0 0 0)
N1C	PDC	N2C	78.92 ± 0.10	(1 0 0 0) (1 0 0 0)
N1C	PDC	C12C	161.64 ± 0.11	(1 0 0 0) (1 0 0 0)
N2C	PDC	C12C	82.87 ± 0.11	(1 0 0 0) (1 0 0 0)
N1A	C1A	1.3338 ± 0.0031	(1 0 0 0)	
N1A	C5A	1.3661 ± 0.0030	(1 0 0 0)	
PDA	N1A	C1A	129.95 ± 0.17	(1 0 0 0) (1 0 0 0)
PDA	N1A	C5A	111.41 ± 0.14	(1 0 0 0) (1 0 0 0)
C1A	N1A	C5A	118.64 ± 0.21	(1 0 0 0) (1 0 0 0)
N2A	C6A	1.3520 ± 0.0031	(1 0 0 0)	
N2A	C10A	1.3497 ± 0.0030	(1 0 0 0)	
PDA	N2A	C6A	118.19 ± 0.15	(1 0 0 0) (1 0 0 0)
PDA	N2A	C10A	118.45 ± 0.16	(1 0 0 0) (1 0 0 0)
C6A	N2A	C10A	122.82 ± 0.20	(1 0 0 0) (1 0 0 0)
N1B	C1B	1.3407 ± 0.0037	(1 0 0 0)	
N1B	C5B	1.3612 ± 0.0036	(1 0 0 0)	

PDB	N1B	C1B	128.73 ± 0.19	(1 0 0 0)	(1 0 0 0)
PDB	N1B	C5B	112.01 ± 0.16	(1 0 0 0)	(1 0 0 0)
C1B	N1B	C5B	119.21 ± 0.23	(1 0 0 0)	(1 0 0 0)
N2B	C6B	1.3495 ± 0.0032	(1 0 0 0)		
N2B	C10B	1.3489 ± 0.0031	(1 0 0 0)		
PDB	N2B	C6B	118.66 ± 0.16	(1 0 0 0)	(1 0 0 0)
PDB	N2B	C10B	117.98 ± 0.17	(1 0 0 0)	(1 0 0 0)
C6B	N2B	C10B	123.02 ± 0.22	(1 0 0 0)	(1 0 0 0)
N1C	C1C	1.3469 ± 0.0030	(1 0 0 0)		
N1C	C5C	1.3569 ± 0.0031	(1 0 0 0)		
PDC	N1C	C1C	128.77 ± 0.17	(1 0 0 0)	(1 0 0 0)
PDC	N1C	C5C	112.46 ± 0.14	(1 0 0 0)	(1 0 0 0)
C1C	N1C	C5C	118.70 ± 0.21	(1 0 0 0)	(1 0 0 0)
N2C	C6C	1.3434 ± 0.0036	(1 0 0 0)		
N2C	C10C	1.3450 ± 0.0034	(1 0 0 0)		
PDC	N2C	C6C	118.75 ± 0.16	(1 0 0 0)	(1 0 0 0)
PDC	N2C	C10C	118.23 ± 0.21	(1 0 0 0)	(1 0 0 0)
C6C	N2C	C10C	122.76 ± 0.24	(1 0 0 0)	(1 0 0 0)
C1A	C2A	1.3661 ± 0.0039	(1 0 0 0)		
N1A	C1A	C2A	122.72 ± 0.24	(1 0 0 0)	(1 0 0 0)
C2A	C3A	1.3704 ± 0.0041	(1 0 0 0)		
C1A	C2A	C3A	119.23 ± 0.25	(1 0 0 0)	(1 0 0 0)
C3A	C4A	1.3900 ± 0.0040	(1 0 0 0)		
C2A	C3A	C4A	119.25 ± 0.26	(1 0 0 0)	(1 0 0 0)
C4A	C5A	1.3777 ± 0.0035	(1 0 0 0)		
C3A	C4A	C5A	118.99 ± 0.24	(1 0 0 0)	(1 0 0 0)
C5A	C6A	1.4712 ± 0.0031	(1 0 0 0)		
N1A	C5A	C4A	121.10 ± 0.21	(1 0 0 0)	(1 0 0 0)
N1A	C5A	C6A	115.24 ± 0.20	(1 0 0 0)	(1 0 0 0)
C4A	C5A	C6A	123.64 ± 0.22	(1 0 0 0)	(1 0 0 0)
C6A	C7A	1.3947 ± 0.0034	(1 0 0 0)		
N2A	C6A	C5A	115.07 ± 0.19	(1 0 0 0)	(1 0 0 0)
N2A	C6A	C7A	119.50 ± 0.21	(1 0 0 0)	(1 0 0 0)
C5A	C6A	C7A	125.43 ± 0.22	(1 0 0 0)	(1 0 0 0)
C7A	C8A	1.3753 ± 0.0037	(1 0 0 0)		
C6A	C7A	C8A	118.71 ± 0.25	(1 0 0 0)	(1 0 0 0)

C7A	C8A	C9A	120.89 ± 0.25	(1 0 0 0)	(1 0 0 0)
C9A	C10A	1.4026 ± 0.0037	(1 0 0 0)		
C8A	C9A	C10A	119.83 ± 0.25	(1 0 0 0)	(1 0 0 0)
C10A	C11A	1.4984 ± 0.0038	(1 0 0 0)		
N2A	C10A	C9A	118.22 ± 0.24	(1 0 0 0)	(1 0 0 0)
N2A	C10A	C11A	113.66 ± 0.21	(1 0 0 0)	(1 0 0 0)
C9A	C10A	C11A	128.04 ± 0.23	(1 0 0 0)	(1 0 0 0)
C11A	C12A	1.5603 ± 0.0037	(1 0 0 0)		
C11A	C13A	1.5293 ± 0.0047	(1 0 0 0)		
C11A	C14A	1.5472 ± 0.0049	(1 0 0 0)		
C10A	C11A	C12A	108.68 ± 0.21	(1 0 0 0)	(1 0 0 0)
C10A	C11A	C13A	111.73 ± 0.25	(1 0 0 0)	(1 0 0 0)
C10A	C11A	C14A	106.46 ± 0.24	(1 0 0 0)	(1 0 0 0)
C12A	C11A	C13A	109.75 ± 0.25	(1 0 0 0)	(1 0 0 0)
C12A	C11A	C14A	110.15 ± 0.24	(1 0 0 0)	(1 0 0 0)
C13A	C11A	C14A	110.00 ± 0.25	(1 0 0 0)	(1 0 0 0)
PDA	C12A	C11A	110.03 ± 0.18	(1 0 0 0)	(1 0 0 0)
C1B	C2B	1.3869 ± 0.0045	(1 0 0 0)		
N1B	C1B	C2B	121.05 ± 0.29	(1 0 0 0)	(1 0 0 0)
C2B	C3B	1.3775 ± 0.0052	(1 0 0 0)		
C1B	C2B	C3B	119.90 ± 0.32	(1 0 0 0)	(1 0 0 0)
C3B	C4B	1.3797 ± 0.0049	(1 0 0 0)		
C2B	C3B	C4B	118.98 ± 0.29	(1 0 0 0)	(1 0 0 0)
C4B	C5B	1.3777 ± 0.0038	(1 0 0 0)		
C3B	C4B	C5B	119.23 ± 0.30	(1 0 0 0)	(1 0 0 0)
C5B	C6B	1.4749 ± 0.0036	(1 0 0 0)		
N1B	C5B	C4B	121.60 ± 0.26	(1 0 0 0)	(1 0 0 0)
N1B	C5B	C6B	115.15 ± 0.22	(1 0 0 0)	(1 0 0 0)
C4B	C5B	C6B	123.25 ± 0.26	(1 0 0 0)	(1 0 0 0)
C6B	C7B	1.3901 ± 0.0039	(1 0 0 0)		
N2B	C6B	C5B	114.70 ± 0.22	(1 0 0 0)	(1 0 0 0)
N2B	C6B	C7B	119.43 ± 0.23	(1 0 0 0)	(1 0 0 0)
C5B	C6B	C7B	125.87 ± 0.23	(1 0 0 0)	(1 0 0 0)
C7B	C8B	1.3797 ± 0.0040	(1 0 0 0)		
C6B	C7B	C8B	118.93 ± 0.26	(1 0 0 0)	(1 0 0 0)
C8B	C9B	1.3862 ± 0.0046	(1 0 0 0)		

C7B	C8B	C9B	120.18 ± 0.27	(1 0 0 0)	(1 0 0 0)
C9B	C10B	1.3860 ± 0.0038	(1 0 0 0)		
C8B	C9B	C10B	119.81 ± 0.26	(1 0 0 0)	(1 0 0 0)
C10B	C11B	1.5014 ± 0.0038	(1 0 0 0)		
N2B	C10B	C9B	118.60 ± 0.25	(1 0 0 0)	(1 0 0 0)
N2B	C10B	C11B	113.32 ± 0.21	(1 0 0 0)	(1 0 0 0)
C9B	C10B	C11B	127.99 ± 0.24	(1 0 0 0)	(1 0 0 0)
C11B	C12B	1.5454 ± 0.0038	(1 0 0 0)		
C11B	C13B	1.5407 ± 0.0041	(1 0 0 0)		
C11B	C14B	1.5342 ± 0.0037	(1 0 0 0)		
C10B	C11B	C12B	109.05 ± 0.21	(1 0 0 0)	(1 0 0 0)
C10B	C11B	C13B	112.84 ± 0.22	(1 0 0 0)	(1 0 0 0)
C10B	C11B	C14B	106.51 ± 0.22	(1 0 0 0)	(1 0 0 0)
C12B	C11B	C13B	110.15 ± 0.23	(1 0 0 0)	(1 0 0 0)
C12B	C11B	C14B	109.26 ± 0.21	(1 0 0 0)	(1 0 0 0)
C13B	C11B	C14B	108.92 ± 0.23	(1 0 0 0)	(1 0 0 0)
PDB	C12B	C11B	108.87 ± 0.17	(1 0 0 0)	(1 0 0 0)
C1C	C2C	1.3701 ± 0.0040	(1 0 0 0)		
N1C	C1C	C2C	122.12 ± 0.24	(1 0 0 0)	(1 0 0 0)
C2C	C3C	1.3793 ± 0.0042	(1 0 0 0)		
C1C	C2C	C3C	119.58 ± 0.25	(1 0 0 0)	(1 0 0 0)
C3C	C4C	1.3828 ± 0.0039	(1 0 0 0)		
C2C	C3C	C4C	118.99 ± 0.26	(1 0 0 0)	(1 0 0 0)
C4C	C5C	1.3865 ± 0.0036	(1 0 0 0)		
C3C	C4C	C5C	119.15 ± 0.25	(1 0 0 0)	(1 0 0 0)
C5C	C6C	1.4790 ± 0.0032	(1 0 0 0)		
N1C	C5C	C4C	121.39 ± 0.21	(1 0 0 0)	(1 0 0 0)
N1C	C5C	C6C	114.92 ± 0.22	(1 0 0 0)	(1 0 0 0)
C4C	C5C	C6C	123.69 ± 0.23	(1 0 0 0)	(1 0 0 0)
C6C	C7C	1.3774 ± 0.0041	(1 0 0 0)		
N2C	C6C	C5C	114.50 ± 0.22	(1 0 0 0)	(1 0 0 0)
N2C	C6C	C7C	120.68 ± 0.23	(1 0 0 0)	(1 0 0 0)
C5C	C6C	C7C	124.83 ± 0.25	(1 0 0 0)	(1 0 0 0)
C7C	C8C	1.3872 ± 0.0044	(1 0 0 0)		
C6C	C7C	C8C	117.58 ± 0.31	(1 0 0 0)	(1 0 0 0)
C8C	C9C	1.3515 ± 0.0058	(1 0 0 0)		

C7C	C8C	C9C	120.95 ± 0.32	(1 0 0 0)	(1 0 0 0)
C9C	C10C	1.3990 ± 0.0048	(1 0 0 0)		
C8C	C9C	C10C	120.49 ± 0.29	(1 0 0 0)	(1 0 0 0)
C10C	C11C	1.5030 ± 0.0053	(1 0 0 0)		
N2C	C10C	C9C	117.52 ± 0.31	(1 0 0 0)	(1 0 0 0)
N2C	C10C	C11C	114.45 ± 0.26	(1 0 0 0)	(1 0 0 0)
C9C	C10C	C11C	127.77 ± 0.27	(1 0 0 0)	(1 0 0 0)
C11C	C12C	1.5578 ± 0.0045	(1 0 0 0)		
C11C	C13C	1.5394 ± 0.0052	(1 0 0 0)		
C11C	C14C	1.5474 ± 0.0052	(1 0 0 0)		
C10C	C11C	C12C	109.03 ± 0.26	(1 0 0 0)	(1 0 0 0)
C10C	C11C	C13C	111.60 ± 0.30	(1 0 0 0)	(1 0 0 0)
C10C	C11C	C14C	106.54 ± 0.30	(1 0 0 0)	(1 0 0 0)
C12C	C11C	C13C	109.92 ± 0.30	(1 0 0 0)	(1 0 0 0)
C12C	C11C	C14C	109.18 ± 0.29	(1 0 0 0)	(1 0 0 0)
C13C	C11C	C14C	110.48 ± 0.31	(1 0 0 0)	(1 0 0 0)
PDC	C12C	C11C	109.80 ± 0.22	(1 0 0 0)	(1 0 0 0)

Intermolecular Contacts

CLA	H3A	2.7671	(1-1 0 0)
CLB	H6A	2.7111	(-1 0-1 0)
CLB	H3B	2.7019	(1-1 0 0)
CLB	H7C	2.8045	(-1 0 1 0)
CLC	H3C	2.6866	(1 1 0 0)

Table S8. - Full list of bond distances and angles for compound 7.

Intramolecular Contacts

PD	CL	2.3138 ± 0.0010	(1 0 0 0)	
PD	N1	2.1384 ± 0.0020	(1 0 0 0)	
PD	N2	2.0462 ± 0.0022	(1 0 0 0)	
PD	C13	2.0216 ± 0.0025	(1 0 0 0)	
CL	PD	N1	96.31 ± 0.10	(1 0 0 0) (1 0 0 0)
CL	PD	N2	174.41 ± 0.10	(1 0 0 0) (1 0 0 0)
CL	PD	C13	88.05 ± 0.10	(1 0 0 0) (1 0 0 0)
N1	PD	N2	79.08 ± 0.10	(1 0 0 0) (1 0 0 0)
N1	PD	C13	175.57 ± 0.10	(1 0 0 0) (1 0 0 0)
N2	PD	C13	96.52 ± 0.10	(1 0 0 0) (1 0 0 0)
N1	C1	1.3481 ± 0.0036	(1 0 0 0)	
N1	C5	1.3421 ± 0.0036	(1 0 0 0)	
PD	N1	C1	127.25 ± 0.20	(1 0 0 0) (1 0 0 0)
PD	N1	C5	113.49 ± 0.17	(1 0 0 0) (1 0 0 0)
C1	N1	C5	119.17 ± 0.23	(1 0 0 0) (1 0 0 0)
N2	C6	1.3636 ± 0.0032	(1 0 0 0)	
N2	C10	1.3464 ± 0.0033	(1 0 0 0)	
PD	N2	C6	115.11 ± 0.17	(1 0 0 0) (1 0 0 0)
PD	N2	C10	125.32 ± 0.17	(1 0 0 0) (1 0 0 0)
C6	N2	C10	119.26 ± 0.23	(1 0 0 0) (1 0 0 0)
C1	C2	1.3781 ± 0.0044	(1 0 0 0)	
N1	C1	C2	121.75 ± 0.31	(1 0 0 0) (1 0 0 0)
C2	C3	1.3619 ± 0.0055	(1 0 0 0)	
C1	C2	C3	119.26 ± 0.31	(1 0 0 0) (1 0 0 0)
C3	C4	1.3877 ± 0.0050	(1 0 0 0)	
C2	C3	C4	119.85 ± 0.31	(1 0 0 0) (1 0 0 0)
C4	C5	1.3898 ± 0.0039	(1 0 0 0)	
C3	C4	C5	118.42 ± 0.30	(1 0 0 0) (1 0 0 0)
C5	C6	1.4897 ± 0.0037	(1 0 0 0)	
N1	C5	C4	121.55 ± 0.25	(1 0 0 0) (1 0 0 0)
N1	C5	C6	115.42 ± 0.22	(1 0 0 0) (1 0 0 0)
C4	C5	C6	123.02 ± 0.26	(1 0 0 0) (1 0 0 0)
C6	C7	1.3725 ± 0.0043	(1 0 0 0)	
N2	C6	C5	115.96 ± 0.24	(1 0 0 0) (1 0 0 0)

C5	C6	C7	121.94 ± 0.24	(1 0 0 0)	(1 0 0 0)
C7	C8	1.3786 ± 0.0047		(1 0 0 0)	
C6	C7	C8	118.77 ± 0.27	(1 0 0 0)	(1 0 0 0)
C8	C9	1.3791 ± 0.0042		(1 0 0 0)	
C7	C8	C9	119.40 ± 0.30	(1 0 0 0)	(1 0 0 0)
C9	C10	1.3927 ± 0.0043		(1 0 0 0)	
C8	C9	C10	119.99 ± 0.29	(1 0 0 0)	(1 0 0 0)
C10	C11	1.4871 ± 0.0038		(1 0 0 0)	
N2	C10	C9	120.28 ± 0.24	(1 0 0 0)	(1 0 0 0)
N2	C10	C11	119.56 ± 0.25	(1 0 0 0)	(1 0 0 0)
C9	C10	C11	120.15 ± 0.24	(1 0 0 0)	(1 0 0 0)
C11	C12	1.5358 ± 0.0037		(1 0 0 0)	
C10	C11	C12	116.91 ± 0.21	(1 0 0 0)	(1 0 0 0)
C12	C13	1.5160 ± 0.0039		(1 0 0 0)	
C12	C14	1.5337 ± 0.0041		(1 0 0 0)	
C12	C15	1.5319 ± 0.0041		(1 0 0 0)	
C11	C12	C13	110.70 ± 0.20	(1 0 0 0)	(1 0 0 0)
C11	C12	C14	107.05 ± 0.21	(1 0 0 0)	(1 0 0 0)
C11	C12	C15	109.83 ± 0.25	(1 0 0 0)	(1 0 0 0)
C13	C12	C14	108.57 ± 0.24	(1 0 0 0)	(1 0 0 0)
C13	C12	C15	111.36 ± 0.22	(1 0 0 0)	(1 0 0 0)
C14	C12	C15	109.22 ± 0.22	(1 0 0 0)	(1 0 0 0)
PD	C13	C12	116.66 ± 0.19	(1 0 0 0)	(1 0 0 0)

Intermolecular Contacts

CL	H4	2.7880	(1-1 0 0)
----	----	--------	------------